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LC Multiresidue Pesticide Standards Kit

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I. INTRODUCTION

The LC Multiresidue Pesticide Standards Kit is a fit-for-purpose collection of 204 compounds designed to eliminate the need for sourcing individual pesticide standards and measure each one manually. It allows scientists to more quickly verify and validate the performance of pesticide screening methods.

- Accurately detects and quantifies pesticides from a wide range of samples by LC-MS/MS
- Contains 204 compounds of interest covering many pesticides listed by government agencies
- Formulated and grouped into 10 ampoules for maximum long term stability
- Quantitatively tested to confirm composition

II. LC MULTIRESIDUE PESTICIDE STANDARDS

The LC Multiresidue Pesticide Standards Kit contains 10 different ampoules with multiple compounds. The ampoules' numbers are given below with the total number of compounds present with concentration in each ampoule along with the solvent in which it is shipped.

Waters LC Multiresidue Pesticide Standards Kit
#186007574
Contains 1 ampoule each:

Description	Concentration	Compound	Total compound in vials
LC Multiresidue Pesticide Standard #1	100 µg/mL	Acetonitrile	13
LC Multiresidue Pesticide Standard #2	100 µg/mL	Acetonitrile	16
LC Multiresidue Pesticide Standard #3	100 µg/mL	Acetonitrile	38
LC Multiresidue Pesticide Standard #4	100 µg/mL	Acetonitrile	63
LC Multiresidue Pesticide Standard #5	100 µg/mL	Acetonitrile	30
LC Multiresidue Pesticide Standard #6	100 µg/mL	Acetonitrile	28
LC Multiresidue Pesticide Standard #7	100 µg/mL	Acetonitrile	7
LC Multiresidue Pesticide Standard #8	100 µg/mL	Acetonitrile	1
LC Multiresidue Pesticide Standard #9	100 µg/mL	Acetonitrile	7
LC Multiresidue Pesticide Standard #10	100 µg/mL	Methanol	1

III. STORAGE AND STABILITY

The standard mix is shipped at ambient temperatures. It is highly recommended that upon receipt, the standard should be refrigerated at 2–8 °C for short term storage and frozen at -15–0 °C for long term storage. The compounds used are stable in the unopened ampoule through the expiration date listed. Standard integrity and stability cannot be guaranteed after opening and should be determined by the user.

After opening the ampoule, it is recommended to transfer the contents to the provided LCMS Certified Amber Max Recovery Vial for use and storage.

Concentration is based upon gravimetric preparation using either a balance whose calibration has been verified daily using NIST traceable weights, and/or dilutions with class A glassware.

It is important to note that the shipping stability uncertainty was obtained under temperature extremes for specific time intervals; therefore, the certified combined stressed uncertainty value should only be applied to the product if it was stored at non-standard temperature conditions up to and including 7 days.

Apply the certified combined unstressed uncertainty value if the product was received under standard shipping conditions. Apply the certified combined stressed uncertainty value if the product was received under non-standard conditions as specified below.

Label conditions	Standard conditions	Non-ctandard conditions
25 °C nominal (room temperature)	<60 °C	≥60 °C up to 7 days
10 °C or colder (refrigerate)	<40 °C	≥40 °C up to 7 days
0 °C or colder (freezer)	<25 °C	≥25 °C up to 7 days

The packages amount is the minimum sample size for which uncertainty is valid.

NOTE: Expiration date valid for unopened ampoule stored in compliance with the recommended conditions.

NOTE: When combining a large number of compounds with different chemical functionalities, mix stability can be an issue. In formulating these standards, we extensively studied the 204 compounds involved, and then grouped them into as few mixes as possible while still ensuring maximum long-term stability and reliability. For quantitative analysis, we recommend analyzing each mix separately to ensure accurate results for every compound.

IV. EXAMPLES OF USING THE STANDARDS

In this work, an LC multiresidue pesticide method was developed for the determination of 204 pesticides using simple sample preparation, followed by UPLC® coupled to tandem quadrupole mass spectrometry.

LC system: Waters® ACQUITY UPLC® H-Class

Column: ACQUITY UPLC BEH C_{18}, 1.7 µm, 2.1 x 100 mm

Column temp.: 45 °C

Injection volume: 10 µL

Flow rate: 0.45 mL/min

Mobile phase A: 10 mM ammonium acetate (pH 5) in water

Mobile phase B: 10 mM ammonium acetate (pH 5) in methanol

Weak needle wash: 50/50 water/methanol (v/v)

Strong needle wash: 10/90 methanol/water (v/v)

Seal wash: 90/10 water/methanol

Gradient:

Time (min)	Flow rate (mL/min)	%A	%B	Curve
Initial	0.450	98	2	6
0.25	0.450	98	2	6
12.25	0.450	1	99	6
13.00	0.450	1	99	6
13.01	0.450	98	2	6
17.00	0.450	98	2	6

MS system: Xevo® TQD

Ionization mode: ESI+

Capillary voltage: 1 kV

Desolvation temp.: 500 °C

Desolvation gas flow: 1000 L/Hr

Source temp.: 150 °C

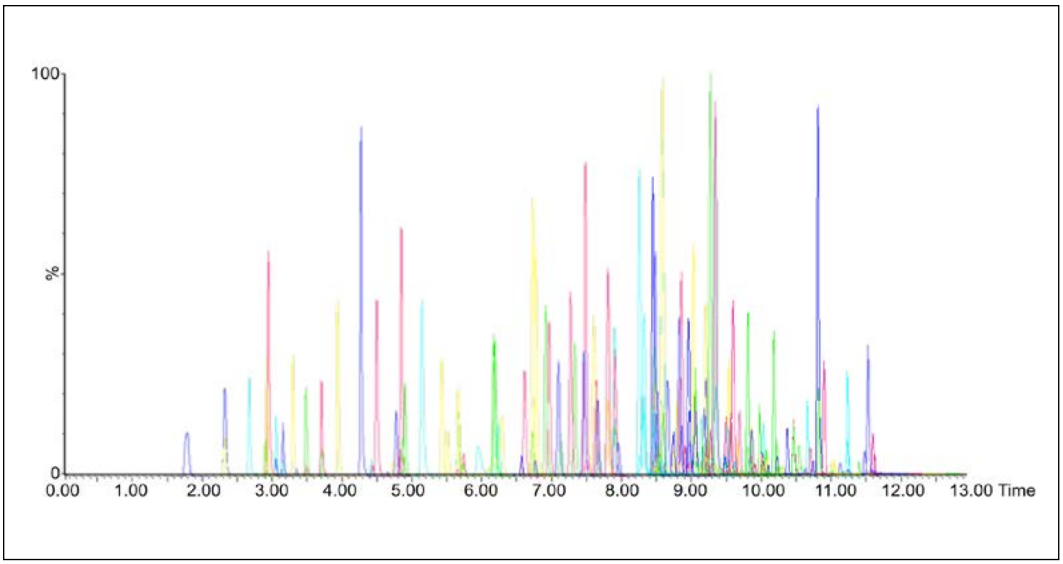

Figure 1. Overlay chromatogram of the 204 pesticides mix at 10 ppb level in 1:1 acetonitrile:water.

All the pesticides of interest were successfully analyzed with a simple sample preparation procedure and UPLC-MS/MS.

The chart below includes the compound name, molecular formula, ion mode (+/- ve), with retention time (RT), precursor, cone voltage (CV), and collision energy (CE), on a Waters UPLC and tandem quadrupole mass spectrometer.

Vial no.	Compound name	Molecular formula	Ion mode	RT	Precursor	CV	Product	CE
1	Acephate	$C_4H_{10}NO_3PS$	ES+	2.19	184.1	20	143.0	10
1	Acephate	$C_4H_{10}NO_3PS$	ES+	2.19	184.1	20	49.0	20
1	Carbaryl	$C_{12}H_{11}NO_2$	ES+	7.17	202.0	20	145.0	10
1	Carbaryl	$C_{12}H_{11}NO_2$	ES+	7.17	202.0	20	117.0	25
1	Dicrotophos	$C_8H_{16}NO_5P$	ES+	4.25	238.0	25	112.0	10
1	Dicrotophos	$C_8H_{16}NO_5P$	ES+	4.25	238.0	25	193.0	10
1	Dimethoate	$C_5H_{12}NO_3PS_2$	ES+	4.72	230.1	20	125.0	10
1	Dimethoate	$C_5H_{12}NO_3PS_2$	ES+	4.72	230.1	20	199.0	20
1	Dimethomorph I	$C_{21}H_{22}ClNO_4$	ES+	8.82	388.1	45	300.9	20
1	Dimethomorph I	$C_{21}H_{22}ClNO_4$	ES+	8.82	388.1	45	165.0	30
1	Dimethomorph II	$C_{21}H_{22}ClNO_4$	ES+	9.10	388.1	45	300.9	20
1	Dimethomorph II	$C_{21}H_{22}ClNO_4$	ES+	9.10	388.1	45	165.0	30
1	Isocarbofos	$C_{11}H_{16}NO_4PS$	ES+	8.06	291.1	20	121.1	30
1	Isocarbofos	$C_{11}H_{16}NO_4PS$	ES+	8.06	291.1	20	231.1	15
1	Methamidophos	$C_2H_8NO_2PS$	ES+	1.67	142.0	30	93.9	15
1	Methamidophos	$C_2H_8NO_2PS$	ES+	1.67	142.0	30	124.9	15
1	Mevinphos I	$C_7H_{13}O_6P$	ES+	4.84	225.1	20	127.1	15
1	Mevinphos I	$C_7H_{13}O_6P$	ES+	4.84	225.1	20	193.1	10
1	Mevinphos II	$C_7H_{13}O_6P$	ES+	5.53	225.1	25	127.1	15
1	Mevinphos II	$C_7H_{13}O_6P$	ES+	5.53	225.1	25	193.1	5
1	Monocrotophos	$C_7H_{14}NO_5P$	ES+	3.89	224.1	25	127.1	15

Vial no.	Compound name	Molecular formula	Ion mode	RT	Precursor	CV	Product	CE
1	Monocrotophos	$C_7H_{14}NO_5P$	ES+	3.89	224.1	25	98.1	10
1	Omethoate	$C_5H_{12}NO_4PS$	ES+	2.52	214.1	25	125.1	20
1	Omethoate	$C_5H_{12}NO_4PS$	ES+	2.52	214.1	25	183.1	10
1	Temephos	$C_{16}H_{20}O_6P_2S_3$	ES+	11.06	466.8	40	125.0	30
1	Temephos	$C_{16}H_{20}O_6P_2S_3$	ES+	11.06	466.8	40	418.9	20
1	Trichlorfon	$C_4H_8Cl_3O_4P$	ES+	4.64	257.0	35	109.0	15
1	Trichlorfon	$C_4H_8Cl_3O_4P$	ES+	4.64	257.0	35	79.0	30
1	Vamidothion	$C_8H_{18}NO_4PS_2$	ES+	4.86	288.0	20	146.0	10
1	Vamidothion	$C_8H_{18}NO_4PS_2$	ES+	4.86	288.0	20	118.0	25
2	Alanycarb	$C_{17}H_{25}N_3O_4S_2$	ES+	9.95	400.1	15	238.1	14
2	Alanycarb	$C_{17}H_{25}N_3O_4S_2$	ES+	9.95	400.1	15	90.9	4
2	Aldicarb	$C_7H_{14}N_2O_2S$	ES+	5.76	213.1	30	89.1	20
2	Aldicarb	$C_7H_{14}N_2O_2S$	ES+	5.76	213.1	30	116.1	10
2	Aldicarb sulfone	$C_7H_{14}N_2O_4S$	ES+	3.04	223.0	30	86.00	15
2	Aldicarb sulfone	$C_7H_{14}N_2O_4S$	ES+	3.04	223.0	30	148.0	10
2	Aldicarb sulfoxide	$C_7H_{14}N_2O_3S$	ES+	2.80	207.0	20	132.0	5
2	Aldicarb sulfoxide	$C_7H_{14}N_2O_3S$	ES+	2.80	207.0	20	89.0	15
2	Benfuracarb	$C_{20}H_{30}N_2O_5S$	ES+	10.77	411.2	15	190.0	23
2	Benfuracarb	$C_{20}H_{30}N_2O_5S$	ES+	10.77	411.2	15	252.1	13
2	Butocarboxim	$C_7H_{14}N_2O_2S$	ES+	5.71	213.0	25	75.0	15
2	Butocarboxim	$C_7H_{14}N_2O_2S$	ES+	5.71	213.0	25	116.0	10
2	Butoxycarboxim	$C_7H_{14}N_2O_4S$	ES+	3.00	223.0	25	106.0	10
2	Butoxycarboxim	$C_7H_{14}N_2O_4S$	ES+	3.00	223.0	25	166.0	5
2	Ethiofencarb	$C_{11}H_{15}NO_2S$	ES+	7.33	226.1	20	107.0	15
2	Ethiofencarb	$C_{11}H_{15}NO_2S$	ES+	7.33	226.1	20	164.0	10
2	Furathiocarb	$C_{18}H_{26}N_2O_5S$	ES+	10.87	383.2	25	194.9	15
2	Furathiocarb	$C_{18}H_{26}N_2O_5S$	ES+	10.87	383.2	25	252.0	10
2	Methabenzthiazuron	$C_{10}H_{11}N_3OS$	ES+	7.72	222.0	30	165.0	15
2	Methabenzthiazuron	$C_{10}H_{11}N_3OS$	ES+	7.72	222.0	30	150.0	30
2	Methiocarb	$C_{11}H_{15}NO_2S$	ES+	8.73	226.0	25	121.0	20
2	Methiocarb	$C_{11}H_{15}NO_2S$	ES+	8.73	226.0	25	169.0	10
2	Methomyl	$C_5H_{10}N_2O_2S$	ES+	3.39	163.0	15	88.0	10
2	Methomyl	$C_5H_{10}N_2O_2S$	ES+	3.39	163.0	15	106.0	10
2	Oxamyl	$C_7H_{13}N_3O_3S$	ES+	3.19	237.0	15	72.0	10
2	Oxamyl	$C_7H_{13}N_3O_3S$	ES+	3.19	237.0	15	90.0	10
2	Tebuthiuron	$C_9H_{16}N_4OS$	ES+	6.98	229.0	35	172.0	15
2	Tebuthiuron	$C_9H_{16}N_4OS$	ES+	6.98	229.0	35	116.0	25
2	Thidiazuron	$C_9H_8N_4OS$	ES+	6.85	221.0	30	101.9	15
2	Thidiazuron	$C_9H_8N_4OS$	ES+	6.85	221.0	30	93.9	15
2	Thiophanate-methyl	$C_{12}H_{14}N_4O_4S_2$	ES+	6.76	343.0	25	151.0	20
2	Thiophanate-methyl	$C_{12}H_{14}N_4O_4S_2$	ES+	6.76	343.0	25	93.0	35

Vial no.	Compound name	Molecular formula	Ion mode	RT	Precursor	CV	Product	CE
3	Bendiocarb	$C_{11}H_{13}NO_4$	ES+	6.78	224.1	25	167.0	10
3	Bendiocarb	$C_{11}H_{13}NO_4$	ES+	6.78	224.1	25	109.0	15
3	Carbofuran	$C_{12}H_{15}NO_3$	ES+	6.78	222.1	25	165.1	10
3	Carbofuran	$C_{12}H_{15}NO_3$	ES+	6.78	222.1	25	123.0	20
3	Carbofuran-3-hydroxy	$C_{12}H_{15}NO_4$	ES+	4.89	238.0	30	181.0	10
3	Carbofuran-3-hydroxy	$C_{12}H_{15}NO_4$	ES+	4.89	238.0	30	163.0	15
3	Chlorfluazuron	$C_{20}H_9Cl_3F_5N_3O_3$	ES+	11.73	539.8	42	158.0	15
3	Chlorfluazuron	$C_{20}H_9Cl_3F_5N_3O_3$	ES+	11.73	539.8	42	382.9	20
3	Chloroxuron	$C_{15}H_{15}ClN_2O_2$	ES+	9.28	291.1	35	72.0	20
3	Chloroxuron	$C_{15}H_{15}ClN_2O_2$	ES+	9.28	291.1	35	164.1	15
3	Chlortoluron	$C_{10}H_{13}ClN_2O$	ES+	7.53	213.0	30	72.0	15
3	Chlortoluron	$C_{10}H_{13}ClN_2O$	ES+	7.53	213.0	30	46.0	15
3	Cycluron	$C_{11}H_{22}N_2O$	ES+	7.96	199.0	35	89.1	15
3	Cycluron	$C_{11}H_{22}N_2O$	ES+	7.96	199.0	35	69.2	20
3	Diethofencarb	$C_{14}H_{21}NO_4$	ES+	8.53	268.0	20	226.0	10
3	Diethofencarb	$C_{14}H_{21}NO_4$	ES+	8.53	268.0	20	124.0	30
3	Diflubenzuron	$C_{14}H_9ClF_2N_2O_2$	ES+	9.69	311.1	20	158.0	10
3	Diflubenzuron	$C_{14}H_9ClF_2N_2O_2$	ES+	9.69	311.1	20	141.0	15
3	Dioxacarb	$C_{11}H_{13}NO_4$	ES+	4.78	224.1	20	123.1	15
3	Dioxacarb	$C_{11}H_{13}NO_4$	ES+	4.78	224.1	20	167.1	10
3	Diuron	$C_9H_{10}Cl_2N_2O$	ES+	7.98	233.0	35	72.1	20
3	Diuron	$C_9H_{10}Cl_2N_2O$	ES+	7.98	233.0	35	46.3	15
3	Fenobucarb	$C_{12}H_{17}NO_2$	ES+	8.53	208.0	25	94.9	15
3	Fenobucarb	$C_{12}H_{17}NO_2$	ES+	8.53	208.0	25	152.0	10
3	Fenoxycarb	$C_{17}H_{19}NO_4$	ES+	9.76	302.1	25	88.0	20
3	Fenoxycarb	$C_{17}H_{19}NO_4$	ES+	9.76	302.1	25	116.1	10
3	Fenuron	$C_9H_{12}N_2O$	ES+	4.48	165.0	30	71.9	15
3	Fenuron	$C_9H_{12}N_2O$	ES+	4.48	165.0	30	45.9	15
3	Flufenoxuron	$C_{21}H_{11}ClF_6N_2O_3$	ES+	11.49	489.1	40	158.0	22
3	Flufenoxuron	$C_{21}H_{11}ClF_6N_2O_3$	ES+	11.49	489.1	40	141.0	46
3	Fluomethuron	$C_{10}H_{11}F_3N_2O$	ES+	7.39	233.2	35	72.2	20
3	Fluomethuron	$C_{10}H_{11}F_3N_2O$	ES+	7.39	233.2	35	46.4	20
3	Forchlorfenuron	$C_{12}H_{10}ClN_3O$	ES+	8.08	248.1	30	129.0	15
3	Forchlorfenuron	$C_{12}H_{10}ClN_3O$	ES+	8.08	248.1	30	93.0	35
3	Indoxacarb	$C_{22}H_{17}ClF_3N_3O_7$	ES+	10.58	528.0	10	150.0	25
3	Indoxacarb	$C_{22}H_{17}ClF_3N_3O_7$	ES+	10.58	528.0	10	203.0	30
3	Iprovalicarb Isomer 1	$C_{18}H_{28}N_2O_3$	ES+	9.16	321.1	20	119.1	20
3	Iprovalicarb Isomer 1	$C_{18}H_{28}N_2O_3$	ES+	9.16	321.1	20	203.1	10
3	Iprovalicarb Isomer 2	$C_{18}H_{28}N_2O_3$	ES+	9.16	321.2	20	119.0	20
3	Iprovalicarb Isomer 2	$C_{18}H_{28}N_2O_3$	ES+	9.16	321.2	20	203.1	10
3	Isoprocarb	$C_{11}H_{15}NO_2$	ES+	7.72	194.1	25	95.1	15

Vial no.	Compound name	Molecular formula	Ion mode	RT	Precursor	CV	Product	CE
3	Isoprocarb	$C_{11}H_{15}NO_2$	ES+	7.72	194.1	25	137.1	10
3	Isoproturon	$C_{12}H_{18}N_2O$	ES+	7.88	207.0	35	72.0	15
3	Isoproturon	$C_{12}H_{18}N_2O$	ES+	7.88	207.0	35	46.1	15
3	Linuron	$C_9H_{10}Cl_2N_2O_2$	ES+	8.60	249.1	30	160.1	20
3	Linuron	$C_9H_{10}Cl_2N_2O_2$	ES+	8.60	249.1	30	182.1	15
3	Lufenuron	$C_{17}H_8Cl_2F_8N_2O_3$	ES+	11.19	511.1	27	158.1	22
3	Lufenuron	$C_{17}H_8Cl_2F_8N_2O_3$	ES+	11.19	511.1	27	141.2	40
3	Metobromuron	$C_9H_{11}BrN_2O_2$	ES+	7.56	259.1	30	170.0	20
3	Metobromuron	$C_9H_{11}BrN_2O_2$	ES+	7.56	259.1	30	148.1	15
3	Monolinuron	$C_9H_{11}ClN_2O_2$	ES+	7.20	215.0	30	126.0	15
3	Monolinuron	$C_9H_{11}ClN_2O_2$	ES+	7.20	215.0	30	99.0	30
3	Neburon	$C_{12}H_{16}Cl_2N_2O$	ES+	9.78	275.0	35	88.0	15
3	Neburon	$C_{12}H_{16}Cl_2N_2O$	ES+	9.78	275.0	35	57.0	20
3	Novaluron	$C_{17}H_9ClF_8N_2O_4$	ES+	10.75	493.0	30	158.0	15
3	Novaluron	$C_{17}H_9ClF_8N_2O_4$	ES+	10.75	493.0	30	141.1	30
3	Pirimicarb	$C_{11}H_{18}N_4O_2$	ES+	7.54	239.1	35	72.0	20
3	Pirimicarb	$C_{11}H_{18}N_4O_2$	ES+	7.54	239.1	35	182.1	15
3	Promecarb	$C_{12}H_{17}NO_2$	ES+	8.90	208.1	25	109.0	15
3	Promecarb	$C_{12}H_{17}NO_2$	ES+	8.90	208.1	25	151.0	10
3	Propham	$C_{10}H_{13}NO_2$	ES+	7.20	180.0	15	138.0	10
3	Propham	$C_{10}H_{13}NO_2$	ES+	7.20	180.0	15	120.0	15
3	Propoxur	$C_{11}H_{15}NO_3$	ES+	6.67	210.0	20	111.0	15
3	Propoxur	$C_{11}H_{15}NO_3$	ES+	6.67	210.0	20	168.0	5
3	Pyraclostrobin	$C_{19}H_{18}ClN_3O_4$	ES+	10.18	388.1	25	163.0	25
3	Pyraclostrobin	$C_{19}H_{18}ClN_3O_4$	ES+	10.18	388.1	25	193.9	10
3	Siduron	$C_{14}H_{20}N_2O$	ES+	8.60	233.0	35	93.8	20
3	Siduron	$C_{14}H_{20}N_2O$	ES+	8.60	233.0	35	137.0	15
3	Teflubenzuron	$C_{14}H_6Cl_2F_4N_2O_2$	ES+	11.15	380.9	30	158.0	20
3	Teflubenzuron	$C_{14}H_6Cl_2F_4N_2O_2$	ES+	11.15	380.9	30	140.9	30
3	Thiobencarb	$C_{12}H_{16}ClNOS$	ES+	10.30	258.1	25	125.0	15
3	Thiobencarb	$C_{12}H_{16}ClNOS$	ES+	10.30	258.1	25	89.0	35
3	Triflumuron	$C_{15}H_{10}ClF_3N_2O_3$	ES+	10.26	359.0	25	156.1	20
3	Triflumuron	$C_{15}H_{10}ClF_3N_2O_3$	ES+	10.26	359.0	25	139.1	30
3	Bifenazate	$C_{17}H_{20}N_2O_3$	ES+	9.28	301.1	15	198.0	10
3	Bifenazate	$C_{17}H_{20}N_2O_3$	ES+	9.28	301.1	15	170.0	20
3	Hexaflumuron	$C_{16}H_8Cl_2F_6N_2O_3$	ES-	10.67	459.1	26	175.0	15
3	Hexaflumuron	$C_{16}H_8Cl_2F_6N_2O_3$	ES-	10.67	459.1	26	276.1	30
4	Abamectin	$C_{49}H_{74}O_{14}$	ES+	12.05	890.6	10	567.4	11
4	Abamectin	$C_{49}H_{74}O_{15}$	ES+	12.05	890.6	10	305.2	25
4	Acetamiprid	$C_{10}H_{11}ClN_4$	ES+	4.92	223.0	35	126.0	20
4	Acetamiprid	$C_{10}H_{11}ClN_4$	ES+	4.92	223.0	35	56.1	15

Vial no.	Compound name	Molecular formula	Ion mode	RT	Precursor	CV	Product	CE
4	Ametryn	$C_9H_{17}N_5S$	ES+	8.57	228.1	40	186.1	20
4	Ametryn	$C_9H_{17}N_5S$	ES+	8.57	228.1	40	68.1	35
4	Azoxystrobin	$C_{22}H_{17}N_3O_5$	ES+	8.67	404.0	25	372.0	25
4	Azoxystrobin	$C_{22}H_{17}N_3O_5$	ES+	8.67	404.0	25	329.0	30
4	Benalaxyl	$C_{20}H_{23}NO_3$	ES+	10.00	326.1	25	148.0	20
4	Benalaxyl	$C_{20}H_{23}NO_3$	ES+	10.00	326.1	25	91.0	30
4	Benzoximate	$C_{18}H_{18}ClNO_5$	ES+	10.28	364.0	15	199.1	10
4	Benzoximate	$C_{18}H_{18}ClNO_5$	ES+	10.28	364.0	15	105.0	25
4	Boscalid	$C_{18}H_{12}Cl_2N_2O$	ES+	8.89	342.9	40	307.0	45
4	Boscalid	$C_{18}H_{12}Cl_2N_2O$	ES+	8.89	342.9	40	139.9	20
4	Butafenacil	$C_{20}H_{18}ClF_3N_2O_6$	ES+	9.31	492.0	25	331.0	25
4	Butafenacil	$C_{20}H_{18}ClF_3N_2O_6$	ES+	9.31	492.0	25	180.0	35
4	Carbetamide	$C_{12}H_{16}N_2O_3$	ES+	6.29	237.0	20	192.0	10
4	Carbetamide	$C_{12}H_{16}N_2O_3$	ES+	6.29	237.0	20	118.0	15
4	Carfentrazone-ethyl	$C_{15}H_{14}Cl_2F_3N_3O_3$	ES+	9.80	412.0	40	346.0	24
4	Carfentrazone-ethyl	$C_{15}H_{14}Cl_2F_3N_3O_3$	ES+	9.80	412.0	40	266.0	18
4	Chlorantraniliprole	$C_{18}H_{14}BrCl_2N_5O_2$	ES+	8.35	484.0	25	453.0	15
4	Chlorantraniliprole	$C_{18}H_{14}BrCl_2N_5O_2$	ES+	8.35	484.0	25	286.0	15
4	Clofentezine	$C_{14}H_8Cl_2N_4$	ES+	10.23	303.0	25	138	15
4	Clofentezine	$C_{14}H_8Cl_2N_4$	ES+	10.23	303.0	25	102.0	35
4	Cymoxanil	$C_7H_{10}N_4O_3$	ES+	5.10	199.0	20	128.0	10
4	Cymoxanil	$C_7H_{10}N_4O_3$	ES+	5.10	199.0	20	111.0	20
4	Cyprodinil	$C_{14}H_{15}N_3$	ES+	9.89	226.0	40	93.0	35
4	Cyprodinil	$C_{14}H_{15}N_3$	ES+	9.89	226.0	40	108.0	25
4	Cyromazine	$C_6H_{10}N_6$	ES+	2.19	167.0	35	60.2	20
4	Cyromazine	$C_6H_{10}N_6$	ES+	2.19	167.0	35	108.1	20
4	Dimoxystrobin	$C_{19}H_{22}N_2O_3$	ES+	9.79	327.1	20	116.1	20
4	Dimoxystrobin	$C_{19}H_{22}N_2O_3$	ES+	9.79	327.1	20	205.2	10
4	Dinotefuran	$C_7H_{14}N_4O_3$	ES+	2.78	203.0	20	129.0	10
4	Dinotefuran	$C_7H_{14}N_4O_3$	ES+	2.78	203.0	20	113.0	10
4	Doramectin	$C_{50}H_{74}O_{14}$	ES+	12.31	916.6	20	331.2	23
4	Doramectin	$C_{50}H_{74}O_{14}$	ES+	12.31	916.6	20	593.4	14
4	Eprinomectin	$C_{50}H_{75}NO_{14}$	ES+	11.91	914.6	20	186.0	35
4	Eprinomectin	$C_{50}H_{75}NO_{14}$	ES+	11.91	914.6	20	144.0	41
4	Famoxadone	$C_{22}H_{18}N_2O_4$	ES+	10.18	392.2	20	331.1	10
4	Famoxadone	$C_{22}H_{18}N_2O_4$	ES+	10.18	392.2	20	238.0	15
4	Fenazaquin	$C_{20}H_{22}N_2O$	ES+	11.80	307.2	20	57.2	20
4	Fenazaquin	$C_{20}H_{22}N_2O$	ES+	11.80	307.2	29	161.0	15
4	Fenhexamid	$C_{14}H_{17}Cl_2NO_2$	ES+	9.37	302.1	45	97.2	25
4	Fenhexamid	$C_{14}H_{17}Cl_2NO_2$	ES+	9.37	302.1	45	55.3	35
4	Fenpyroximat	$C_{24}H_{27}N_3O_4$	ES+	11.56	422.2	15	366.1	20

Vial no.	Compound name	Molecular formula	Ion mode	RT	Precursor	CV	Product	CE
4	Fenpyroximat	$C_{24}H_{27}N_3O_4$	ES+	11.56	422.2	15	138.1	30
4	Flonicamid	$C_9H_6F_3N_3O$	ES+	3.42	230.0	40	203.0	15
4	Flonicamid	$C_9H_6F_3N_3O$	ES+	3.42	230.0	40	148.0	25
4	Fluoxastrobin	$C_{21}H_{16}ClFN_4O_5$	ES+	9.37	459.0	35	427.0	15
4	Fluoxastrobin	$C_{21}H_{16}ClFN_4O_5$	ES+	9.37	459.0	35	188.0	35
4	Flutolanil	$C_{17}H_{16}F_3NO_2$	ES+	8.99	324.1	35	262.1	20
4	Flutolanil	$C_{17}H_{16}F_3NO_2$	ES+	8.99	324.1	35	65.0	35
4	Furalaxyl	$C_{17}H_{19}NO_4$	ES+	8.65	302.1	25	95	25
4	Furalaxyl	$C_{17}H_{19}NO_4$	ES+	8.65	302.1	25	242.1	15
4	Halofenzoide	$C_{18}H_{19}ClN_2O_2$	ES+	8.76	331.1	10	104.9	15
4	Halofenzoide	$C_{18}H_{19}ClN_2O_2$	ES+	8.76	331.1	10	275.0	5
4	Imazalil	$C_{14}H_{14}Cl_2N_2O$	ES+	9.65	297.0	40	159.0	20
4	Imazalil	$C_{14}H_{14}Cl_2N_2O$	ES+	9.65	297.0	40	69.0	20
4	Imidacloprid	$C_9H_{10}ClN_5O_2$	ES+	4.41	256.1	30	175.1	20
4	Imidacloprid	$C_9H_{10}ClN_5O_2$	ES+	4.41	256.1	30	209.1	15
4	Ivermectine	$C_{48}H_{74}O_{14}$	ES+	12.63	892.6	20	551.4	25
4	Ivermectine	$C_{48}H_{74}O_{14}$	ES+	12.63	892.6	20	569.4	14
4	Kresoxim-methyl	$C_{18}H_{19}NO_4$	ES+	9.82	314.1	15	116.0	15
4	Kresoxim-methyl	$C_{18}H_{19}NO_4$	ES+	9.82	314.1	15	206.0	5
4	Mandipropamid	$C_{23}H_{22}ClNO_4$	ES+	8.95	412.0	30	328.0	15
4	Mandipropamid	$C_{23}H_{22}ClNO_4$	ES+	8.95	412.0	30	125.0	35
4	Mepanipyrim	$C_{14}H_{13}N_3$	ES+	9.22	224.1	50	106.0	25
4	Mepanipyrim	$C_{14}H_{13}N_3$	ES+	9.22	224.1	50	77.0	35
4	Mepronil	$C_{17}H_{19}NO_2$	ES+	8.99	270.1	35	119.0	25
4	Mepronil	$C_{17}H_{19}NO_2$	ES+	8.99	270.1	35	91.0	35
4	Metalaxyl	$C_{15}H_{21}NO_4$	ES+	7.98	280.1	25	220.1	15
4	Metalaxyl	$C_{15}H_{21}NO_4$	ES+	7.98	280.1	25	192.1	20
4	Methoxyfenozide	$C_{22}H_{28}N_2O_3$	ES+	9.06	369.1	15	149.1	15
4	Methoxyfenozide	$C_{22}H_{28}N_2O_3$	ES+	9.06	369.1	15	313.2	10
4	Moxidectin	$C_{37}H_{53}NO_8$	ES+	12.38	640.5	22	528.4	10
4	Moxidectin	$C_{37}H_{53}NO_8$	ES+	12.38	640.5	22	498.3	10
4	Myclobutanil	$C_{15}H_{17}ClN_4$	ES+	9.20	289.1	35	124.9	30
4	Myclobutanil	$C_{15}H_{17}ClN_4$	ES+	9.20	289.1	35	150.9	25
4	Nitenpyram	$C_{11}H_{15}ClN_4O_2$	ES+	3.25	271.1	30	125.9	30
4	Nitenpyram	$C_{11}H_{15}ClN_4O_2$	ES+	3.25	271.1	30	224.9	10
4	Oxadixyl	$C_{14}H_{18}N_2O_4$	ES+	6.34	279.0	25	219.0	10
4	Oxadixyl	$C_{14}H_{18}N_2O_4$	ES+	6.34	279.0	25	132.0	30
4	Picoxystrobin	$C_{18}H_{16}F_3NO_4$	ES+	9.73	368.0	15	145.1	25
4	Picoxystrobin	$C_{18}H_{16}F_3NO_4$	ES+	9.73	368.0	15	205.1	10
4	Piperonyl butoxide	$C_{19}H_{30}O_5$	ES+	11.00	356.3	20	176.9	10
4	Piperonyl butoxide	$C_{19}H_{30}O_5$	ES+	11.00	356.3	20	119.0	35

Vial no.	Compound name	Molecular formula	Ion mode	RT	Precursor	CV	Product	CE
4	Procloraz	$C_{15}H_{16}Cl_3N_3O_2$	ES+	10.27	376.0	35	307.1	15
4	Procloraz	$C_{15}H_{16}Cl_3N_3O_2$	ES+	10.27	376.0	35	70.1	25
4	Prometon	$C_{10}H_{19}N_5O$	ES+	8.38	226.0	40	86.3	30
4	Prometon	$C_{10}H_{19}N_5O$	ES+	8.38	226.0	40	184.3	20
4	Pymetrozine	$C_{10}H_{11}N_5O$	ES+	3.66	218.0	35	105.0	20
4	Pymetrozine	$C_{10}H_{11}N_5O$	ES+	3.66	218.0	35	79.0	35
4	Pyracarbolid	$C_{13}H_{15}NO_2$	ES+	6.83	218.1	30	125.1	20
4	Pyracarbolid	$C_{13}H_{15}NO_2$	ES+	6.83	218.1	30	97.1	30
4	Pyrimethanil	$C_{12}H_{13}N_3$	ES+	8.58	200.0	40	107.0	25
4	Pyrimethanil	$C_{12}H_{13}N_3$	ES+	8.58	200.0	40	82.0	25
4	Pyriproxifen	$C_{20}H_{19}NO_3$	ES+	11.10	322.1	25	96.0	15
4	Pyriproxifen	$C_{20}H_{19}NO_3$	ES+	11.10	322.1	25	227.1	10
4	Quinoxyfen	$C_{15}H_8Cl_2FNO$	ES+	11.22	308.0	61	197.0	30
4	Quinoxyfen	$C_{15}H_8Cl_2FNO$	ES+	11.22	308.0	61	161.9	35
4	Rotenone	$C_{23}H_{22}O_6$	ES+	9.70	395.0	46	213.1	25
4	Rotenone	$C_{23}H_{22}O_6$	ES+	9.70	395.0	46	192.1	20
4	Secbumeton	$C_{10}H_{19}N_5O$	ES+	8.33	226.2	40	170.2	20
4	Secbumeton	$C_{10}H_{19}N_5O$	ES+	8.33	226.2	40	100.2	25
4	Spiroxamine Isomer 1	$C_{18}H_{35}NO_2$	ES+	9.35	298.0	35	144.0	20
4	Spiroxamine Isomer 1	$C_{18}H_{35}NO_2$	ES+	9.35	298.0	35	100.0	30
4	Spiroxamine Isomer 2	$C_{18}H_{35}NO_2$	ES+	9.35	298.2	35	144.2	20
4	Spiroxamine Isomer 2	$C_{18}H_{35}NO_2$	ES+	9.35	298.2	35	100.1	30
4	Tebufenozide	$C_{22}H_{28}N_2O_2$	ES+	9.73	353.1	15	133.0	20
4	Tebufenozide	$C_{22}H_{28}N_2O_2$	ES+	9.73	353.1	15	297.1	10
4	Tebufenpyrad	$C_{18}H_{24}ClN_3O$	ES+	10.94	334.0	40	117.0	25
4	Tebufenpyrad	$C_{18}H_{24}ClN_3O$	ES+	10.94	334.0	40	145.0	25
4	Terbumeton	$C_{10}H_{19}N_5O$	ES+	8.67	226.1	35	170.1	15
4	Terbumeton	$C_{10}H_{19}N_5O$	ES+	8.67	226.1	35	114.1	25
4	Triadimefon	$C_{14}H_{16}ClN_3O_2$	ES+	9.07	294.1	30	69.3	20
4	Triadimefon	$C_{14}H_{16}ClN_3O_2$	ES+	9.07	294.1	30	197.2	15
4	Trifloxystrobin	$C_{20}H_{19}F_3N_2O_4$	ES+	10.55	409.0	34	186.0	16
4	Trifloxystrobin	$C_{20}H_{19}F_3N_2O_4$	ES+	10.55	409.0	34	145.0	40
4	Zoxamide	$C_{14}H_{16}Cl_3NO_2$	ES+	10.05	336.0	35	187.1	20
4	Zoxamide	$C_{14}H_{16}Cl_3NO_2$	ES+	10.05	336.0	35	159.0	35
4	Fluazinam I	$C_{13}H_4Cl_2F_6N_4O_4$	ES-	11.69	462.7	32	415.7	47
4	Fluazinam I	$C_{13}H_4Cl_2F_6N_4O_4$	ES-	11.69	462.7	32	397.8	26
4	Fluazinam 1+	$C_{13}H_4Cl_2F_6N_4O_4$	ES+	11.69	465.0	32	148.9	47
4	Fluazinam 1+	$C_{13}H_4Cl_2F_6N_4O_4$	ES+	11.69	465.0	32	91.0	26
4	Fludioxonil	$C_{12}H_6F_2N_2O_2$	ES-	8.91	247.0	16	180.0	10
4	Fludioxonil	$C_{12}H_6F_2N_2O_2$	ES-	8.91	247.0	16	126.0	15
4	Metaflumizone	$C_{24}H_{16}F_6N_4O_2$	ES-	11.10	507.1	10	178.1	15

Vial no.	Compound name	Molecular formula	Ion mode	RT	Precursor	CV	Product	CE
4	Metaflumizone	$C_{24}H_{16}F_6N_4O_2$	ES-	11.10	507.1	10	287.1	25
4	Amitraz	$C_{19}H_{23}N_3$	ES+	11.72	294.2	15	148.3	25
4	Amitraz	$C_{19}H_{23}N_3$	ES+	11.72	294.2	15	91.2	35
4	Avermectin B1b.1	$C_{48}H_{72}O_{14}$	ES+	11.53	876.5	15	553.4	20
4	Avermectin B1b.2	$C_{48}H_{72}O_{14}$	ES+	11.53	876.5	15	291	30
4	Avermectin B1a.1	$C_{48}H_{72}O_{14}$	ES+	11.53	890.5	15	567.5	20
4	Avermectin B1a.2	$C_{48}H_{72}O_{14}$	ES+	11.53	890.5	15	305	35
5	Acibenzolar-S-methyl	$C_8H_6N_2OS_2$	ES+	8.53	210.9	40	135.9	30
5	Acibenzolar-S-methyl	$C_8H_6N_2OS_2$	ES+	8.53	210.9	40	69.0	35
5	Bupirimate	$C_{13}H_{24}N_4O_3S$	ES+	9.69	317.0	40	166.0	25
5	Bupirimate	$C_{13}H_{24}N_4O_3S$	ES+	9.69	317.0	40	108.0	25
5	Buprofezin	$C_{16}H_{23}N_3OS$	ES+	11.02	306.1	25	201.0	10
5	Buprofezin	$C_{16}H_{23}N_3OS$	ES+	11.02	306.1	25	57.4	25
5	Carboxin	$C_{12}H_{13}NO_2S$	ES+	7.03	236.0	30	143.0	15
5	Carboxin	$C_{12}H_{13}NO_2S$	ES+	7.03	236.0	30	87.0	25
5	Clethodim I	$C_{17}H_{26}ClNO_3S$	ES+	8.21	360.0	25	164.0	20
5	Clethodim I	$C_{17}H_{26}ClNO_3S$	ES+	8.21	360.0	25	268.1	10
5	Clethodim II	$C_{17}H_{26}ClNO_3S$	ES+	9.57	360.0	25	164.0	20
5	Clethodim II	$C_{17}H_{26}ClNO_3S$	ES+	9.57	360.0	25	268.1	10
5	Clothianidin	$C_6H_8ClN_5O_2S$	ES+	4.44	250.0	25	169.0	10
5	Clothianidin	$C_6H_8ClN_5O_2S$	ES+	4.44	250.0	25	132.0	15
5	Cyazofamid	$C_{13}H_{13}ClN_4O_2S$	ES+	9.56	325.0	25	107.9	15
5	Cyazofamid	$C_{13}H_{13}ClN_4O_2S$	ES+	9.56	325.0	25	261.0	10
5	Ethiprole	$C_{13}H_9Cl_2F_3N_4OS$	ES+	8.87	414.1	15	350.9	25
5	Ethiprole	$C_{13}H_9Cl_2F_3N_4OS$	ES+	8.87	414.1	15	396.9	10
5	Ethofumesate	$C_{13}H_{18}O_5S$	ES+	8.60	287.1	35	121.1	15
5	Ethofumesate	$C_{13}H_{18}O_5S$	ES+	8.60	287.1	35	259.1	10
5	Fenamidone	$C_{17}H_{17}N_3OS$	ES+	8.80	312.1	25	92.0	25
5	Fenamidone	$C_{17}H_{17}N_3OS$	ES+	8.80	312.1	25	236.1	15
5	Fipronil	$C_{12}H_4Cl_2F_6N_4OS$	ES+	9.75	453.9	20	368.1	25
5	Fipronil	$C_{12}H_4Cl_2F_6N_4OS$	ES+	9.75	437.1	20	290.0	25
5	Flubendiamide	$C_{23}H_{22}F_7IN_2O_4S$	ES+	9.90	683.0	10	408.0	5
5	Flubendiamide	$C_{23}H_{22}F_7IN_2O_4S$	ES+	9.90	683.0	10	274.0	30
5	Flufenacet	$C_{14}H_{13}F_4N_3O_2S$	ES+	9.37	364.0	25	152.1	20
5	Flufenacet	$C_{14}H_{13}F_4N_3O_2S$	ES+	9.37	364.0	25	194.1	10
5	Hexythiazox	$C_{17}H_{21}ClN_2O_2S$	ES+	11.25	353.0	25	168.1	25
5	Hexythiazox	$C_{17}H_{21}ClN_2O_2S$	ES+	11.25	353.0	25	228.1	15
5	Mefenacet	$C_{16}H_{14}N_2O_2S$	ES+	9.16	299.0	25	148.0	15
5	Mefenacet	$C_{16}H_{14}N_2O_2S$	ES+	9.16	299.0	25	120.0	25
5	Mesotrione	$C_{14}H_{13}NO_7S$	ES+	3.03	340.1	35	228.1	15
5	Mesotrione	$C_{14}H_{13}NO_7S$	ES+	3.03	340.1	35	104.0	30

Vial no.	Compound name	Molecular formula	Ion mode	RT	Precursor	CV	Product	CE
5	Methoprotryne	$C_{11}H_{21}N_5OS$	ES+	8.54	272.2	45	170.2	30
5	Methoprotryne	$C_{11}H_{21}N_5OS$	ES+	8.54	272.2	45	198.2	25
5	Metribuzin	$C_8H_{14}N_4OS$	ES+	6.50	215.0	35	89.0	20
5	Metribuzin	$C_8H_{14}N_4OS$	ES+	6.50	215.0	35	131.0	20
5	Prometryn	$C_{10}H_{19}N_5S$	ES+	9.29	242.0	40	158.0	25
5	Prometryn	$C_{10}H_{19}N_5S$	ES+	9.29	242.0	40	200.1	20
5	Propargite	$C_{19}H_{26}O_4S$	ES+	11.42	368.2	15	231.1	10
5	Propargite	$C_{19}H_{26}O_4S$	ES+	11.42	368.2	15	175.1	15
5	Prothioconazole	$C_{14}H_{15}Cl_2N_3OS$	ES+	10.05	344.0	25	326.0	10
5	Prothioconazole	$C_{14}H_{15}Cl_2N_3OS$	ES+	10.05	344.0	25	189.0	20
5	Pyridaben	$C_{19}H_{25}ClN_2OS$	ES+	11.83	365.1	10	147.1	25
5	Pyridaben	$C_{19}H_{25}ClN_2OS$	ES+	11.83	365.1	10	309.1	10
5	Simetryn	$C_8H_{15}N_5S$	ES+	7.69	214.0	40	124.0	20
5	Simetryn	$C_8H_{15}N_5S$	ES+	7.69	214.0	40	95.9	25
5	Sulfentrazone	$C_{11}H_{10}Cl_2F_2N_4O_3S$	ES+	7.14	387.0	50	145.8	35
5	Sulfentrazone	$C_{11}H_{10}Cl_2F_2N_4O_3S$	ES+	7.14	387.0	50	307.0	30
5	Terbutryn	$C_{10}H_{19}N_5S$	ES+	9.43	242.1	35	186.1	20
5	Terbutryn	$C_{10}H_{19}N_5S$	ES+	9.43	242.1	35	91.0	25
5	Thiabendazole	$C_{10}H_7N_3S$	ES+	5.97	202.0	50	175.0	25
5	Thiabendazole	$C_{10}H_7N_3S$	ES+	5.97	202.0	50	131.0	30
5	Thiacloprid	$C_{10}H_9ClN_4S$	ES+	5.46	253.0	35	126.0	20
5	Thiacloprid	$C_{10}H_9ClN_4S$	ES+	5.46	253.0	35	90.1	35
5	Thiamethoxam	$C_8H_{10}ClN_5O_3S$	ES+	3.66	292.0	25	211.2	10
5	Thiamethoxam	$C_8H_{10}ClN_5O_3S$	ES+	3.66	292.0	25	132.0	20
5	Thiofanox	$C_9H_{18}N_2O_2S$	ES+	7.42	219.0	10	57.0	5
5	Thiofanox	$C_9H_{18}N_2O_2S$	ES+	7.42	219.0	10	76.0	5
5	Tricyclazole	$C_9H_7N_3S$	ES+	5.71	190.0	50	163.0	20
5	Tricyclazole	$C_9H_7N_3S$	ES+	5.71	190.0	50	136.0	25
6	Bitertanol	$C_{20}H_{23}N_3O_2$	ES+	10.30	338.1	15	99.1	15
6	Bitertanol	$C_{20}H_{23}N_3O_2$	ES+	10.30	338.1	15	70.1	10
6	Bromuconazole I	$C_{13}H_{12}BrCl_2N_3O$	ES+	9.17	376.0	40	158.9	30
6	Bromuconazole I	$C_{13}H_{12}BrCl_2N_3O$	ES+	9.17	376.0	40	70.1	20
6	Bromuconazole II	$C_{13}H_{12}BrCl_2N_3O$	ES+	9.83	376.0	40	158.9	45
6	Bromuconazole II	$C_{13}H_{12}BrCl_2N_3O$	ES+	9.83	376.0	40	70.1	40
6	Cyproconazole I	$C_{15}H_{18}ClN_3O$	ES+	9.04	292.2	35	70.2	20
6	Cyproconazole I	$C_{15}H_{18}ClN_3O$	ES+	9.04	292.2	35	125.1	30
6	Cyproconazole II	$C_{15}H_{18}ClN_3O$	ES+	9.30	292.2	35	70.2	20
6	Cyproconazole II	$C_{15}H_{18}ClN_3O$	ES+	9.30	292.2	35	125.1	30
6	Diclobutrazol	$C_{15}H_{19}Cl_2N_3O$	ES+	9.85	328.0	35	70.0	20
6	Diclobutrazol	$C_{15}H_{19}Cl_2N_3O$	ES+	9.85	328.0	35	158.9	35
6	Difenoconazole Isomer 1	$C_{19}H_{17}Cl_2N_3O_3$	ES+	10.47	406.0	40	251.1	25

Vial no.	Compound name	Molecular formula	Ion mode	RT	Precursor	CV	Product	CE
6	Difenoconazole Isomer 1	$C_{19}H_{17}Cl_2N_3O_3$	ES+	10.47	406.0	40	111.1	35
6	Difenoconazole Isomer 2	$C_{19}H_{17}Cl_2N_3O_3$	ES+	10.47	408.2	40	253.1	25
6	Difenoconazole Isomer 2	$C_{19}H_{17}Cl_2N_3O_3$	ES+	10.47	408.2	40	251.1	35
6	Diniconazole	$C_{15}H_{17}Cl_2N_3O$	ES+	10.45	326.1	40	70.2	25
6	Diniconazole	$C_{15}H_{17}Cl_2N_3O$	ES+	10.45	326.1	40	159.0	30
6	Epoxiconazole	$C_{17}H_{13}ClFN_3O$	ES+	9.48	330.0	35	121.0	20
6	Epoxiconazole	$C_{17}H_{13}ClFN_3O$	ES+	9.48	330.0	35	101.0	35
6	Etaconazole isomer 1	$C_{14}H_{15}Cl_2N_3O_2$	ES+	9.43	328.1	35	159.0	25
6	Etaconazole isomer 1	$C_{14}H_{15}Cl_2N_3O_2$	ES+	9.43	328.1	35	205.0	15
6	Etaconazole isomer 2	$C_{14}H_{15}Cl_2N_3O_2$	ES+	9.43	328.1	35	159.0	25
6	Etaconazole isomer 2	$C_{14}H_{15}Cl_2N_3O_2$	ES+	9.43	328.1	35	205.0	15
6	Ethirimol	$C_{11}H_{19}N_3O$	ES+	7.87	210.1	40	140.0	20
6	Ethirimol	$C_{11}H_{19}N_3O$	ES+	7.87	210.1	40	98.0	25
6	Etoxazole	$C_{21}H_{23}F_2NO_2$	ES+	11.42	360.1	31	57.2	25
6	Etoxazole	$C_{21}H_{23}F_2NO_2$	ES+	11.42	360.1	31	141.0	25
6	Fenarimol	$C_{17}H_{12}Cl_2N_2O$	ES+	9.45	331.0	40	81.0	30
6	Fenarimol	$C_{17}H_{12}Cl_2N_2O$	ES+	9.45	331.0	40	268.0	25
6	Fenbuconazole	$C_{19}H_{17}ClN_4$	ES+	9.67	337.0	35	70.1	20
6	Fenbuconazole	$C_{19}H_{17}ClN_4$	ES+	9.67	337.0	35	125.0	30
6	Fluquinconazole	$C_{16}H_8Cl_2FN_5O$	ES+	9.29	376.0	40	306.9	25
6	Fluquinconazole	$C_{16}H_8Cl_2FN_5O$	ES+	9.29	376.0	40	348.8	20
6	Flusilazole	$C_{16}H_{15}F_2N_3Si$	ES+	9.74	316.0	40	247.0	20
6	Flusilazole	$C_{16}H_{15}F_2N_3Si$	ES+	9.74	316.0	40	165.0	25
6	Flutriafol	$C_{16}H_{13}F_2N_3O$	ES+	7.90	302.1	35	70.2	15
6	Flutriafol	$C_{16}H_{13}F_2N_3O$	ES+	7.90	302.1	35	123.1	30
6	Fuberidazole	$C_{11}H_8N_2O$	ES+	6.27	185.0	45	157.0	20
6	Fuberidazole	$C_{11}H_8N_2O$	ES+	6.27	185.0	45	156.0	25
6	Hexaconazole	$C_{14}H_{17}Cl_2N_3O$	ES+	10.23	314.0	35	70.1	20
6	Hexaconazole	$C_{14}H_{17}Cl_2N_3O$	ES+	10.23	314.0	35	159.0	25
6	Ipconazole Isomer 1	$C_{18}H_{24}ClN_3O$	ES+	10.70	334.2	40	70.0	25
6	Ipconazole Isomer 1	$C_{18}H_{24}ClN_3O$	ES+	10.70	334.2	40	125.0	25
6	Ipconazole Isomer 2	$C_{18}H_{24}ClN_3O$	ES+	10.70	334.2	40	70.0	25
6	Ipconazole Isomer 2	$C_{18}H_{24}ClN_3O$	ES+	10.70	334.2	40	125.0	25
6	Metconazole	$C_{17}H_{22}ClN_3O$	ES+	10.24	320.1	35	70.0	25
6	Metconazole	$C_{17}H_{22}ClN_3O$	ES+	10.24	320.1	35	125.0	30
6	Nuarimol	$C_{17}H_{12}ClFN_2O$	ES+	8.72	315.0	40	81.1	15
6	Nuarimol	$C_{17}H_{12}ClFN_2O$	ES+	8.72	315.0	40	252.0	20
6	Paclobutrazol	$C_{30}H_{40}Cl_2N_6O_2$	ES+	8.96	294.1	30	125.1	35
6	Paclobutrazol	$C_{30}H_{40}Cl_2N_6O_2$	ES+	8.96	294.1	30	70.2	20
6	Penconazole	$C_{13}H_{15}Cl_2N_3$	ES+	9.95	284.0	30	70.1	15
6	Penconazole	$C_{13}H_{15}Cl_2N_3$	ES+	9.95	284.0	30	159.0	25

Vial no.	Compound name	Molecular formula	Ion mode	RT	Precursor	CV	Product	CE
6	Propiconazole Isomer 1	$C_{15}H_{17}Cl_2N_3O_2$	ES+	10.06	342.0	40	69.0	20
6	Propiconazole Isomer 1	$C_{15}H_{17}Cl_2N_3O_2$	ES+	10.06	342.0	40	159.0	25
6	Propiconazole Isomer 2	$C_{15}H_{17}Cl_2N_3O_2$	ES+	10.06	342.1	40	159.0	20
6	Propiconazole Isomer 2	$C_{15}H_{17}Cl_2N_3O_2$	ES+	10.06	342.1	40	69.0	25
6	Tebuconazole	$C_{16}H_{22}ClN_3O$	ES+	9.99	308.0	35	70.1	20
6	Tebuconazole	$C_{16}H_{22}ClN_3O$	ES+	9.99	308.0	35	125.0	35
6	Tetraconazole	$C_{13}H_{11}Cl_2F_4N_3O$	ES+	9.50	372.0	40	70.1	20
6	Tetraconazole	$C_{13}H_{11}Cl_2F_4N_3O$	ES+	9.50	372.0	40	159.0	25
6	Triadimenol	$C_{14}H_{18}ClN_3O_2$	ES+	9.27	296.1	20	70.2	10
6	Triadimenol	$C_{14}H_{18}ClN_3O_2$	ES+	9.27	296.1	20	227.1	10
6	Triflumizole	$C_{15}H_{15}ClF_3N_3O$	ES+	10.71	346.0	20	277.9	20
6	Triflumizole	$C_{15}H_{15}ClF_3N_3O$	ES+	10.71	346.0	20	73.1	15
6	Triticonazole	$C_{17}H_{20}ClN_3O$	ES+	9.45	318.1	30	70.1	20
6	Triticonazole	$C_{17}H_{20}ClN_3O$	ES+	9.45	318.1	30	124.9	30
7	Emamectin-benzoate b1b.1	$C_{49}H_{75}NO_{13}$	ES+	11.45	886.6	10	158.0	35
7	Emamectin-benzoate b1b.2	$C_{49}H_{75}NO_{13}$	ES+	11.45	886.6	10	126.0	30
7	Emamectin-benzoate b1a.1	$C_{49}H_{75}NO_{13}$	ES+	11.45	872.6	10	158.2	35
7	Emamectin-benzoate b1a.2	$C_{49}H_{75}NO_{13}$	ES+	11.45	872.6	10	302.3	30
7	Fenpropimorph	$C_{20}H_{33}NO$	ES+	11.66	304.2	50	147.1	30
7	Fenpropimorph	$C_{20}H_{33}NO$	ES+	11.66	304.2	50	57.2	30
7	Spinetoram	$C_{42}H_{69}NO_{10}$	ES+	11.65	748.5	25	142.2	30
7	Spinetoram	$C_{42}H_{69}NO_{10}$	ES+	11.65	748.5	25	98.1	35
7	Spinosad A	$C_{41}H_{65}NO_{10}$	ES+	11.29	732.6	40	142.0	30
7	Spinosad A	$C_{41}H_{65}NO_{10}$	ES+	11.29	732.6	40	98.1	35
7	Spinosad D	$C_{41}H_{65}NO_{10}$	ES+	11.66	746.5	20	142.0	30
7	Spinosad D	$C_{41}H_{65}NO_{10}$	ES+	11.66	746.5	20	98.1	35
7	Spirodiclofen	$C_{21}H_{24}Cl_2O_4$	ES+	11.59	411.1	25	71.2	15
7	Spirodiclofen	$C_{21}H_{24}Cl_2O_4$	ES+	11.59	411.1	25	313.0	10
7	Spiromesifen	$C_{23}H_{30}O_4$	ES+	11.37	371.1	20	273.1	5
7	Spiromesifen	$C_{23}H_{30}O_4$	ES+	11.37	371.1	20	255.1	25
7	Spirotetramat	$C_{21}H_{27}NO_5$	ES+	9.37	374.0	35	302.0	30
7	Spirotetramat	$C_{21}H_{27}NO_5$	ES+	9.37	374.0	35	330.0	15
8	Hydramethylnon	$C_{25}H_{24}F_6N_4$	ES+	10.89	495.1	30	323.2	30
8	Hydramethylnon	$C_{25}H_{24}F_6N_4$	ES+	10.89	495.1	30	151.1	35
9	Aminocarb	$C_{11}H_{16}N_2O_2$	ES+	6.21	209.0	30	137.0	25
9	Aminocarb	$C_{11}H_{16}N_2O_2$	ES+	6.21	209.0	30	152.0	15
9	Desmedipham	$C_{16}H_{16}N_2O_4$	ES+	8.21	301.0	30	182.0	10
9	Desmedipham	$C_{16}H_{16}N_2O_4$	ES+	8.21	301.0	30	136.0	25
9	Formetanate HCL	$C_{11}H_{15}N_3O_2 . HCl$	ES+	2.65	222.0	30	165.0	15
9	Formetanate HCL	$C_{11}H_{15}N_3O_2 . HCl$	ES+	2.65	222.0	30	46.0	25
9	Mexacarbate	$C_{12}H_{18}N_2O_2$	ES+	8.93	223.2	30	166.1	15

Vial no.	Compound name	Molecular formula	Ion mode	RT	Precursor	CV	Product	CE
9	Mexacarbate	$C_{12}H_{18}N_2O_2$	ES+	8.93	223.2	30	151.0	25
9	(Monceren) Pencycuron	$C_{19}H_{21}ClN_2O$	ES+	10.40	329.1	35	218.0	15
9	(Monceren) Pencycuron	$C_{19}H_{21}ClN_2O$	ES+	10.40	329.1	35	125.0	25
9	Phenmedipham	$C_{16}H_{16}N_2O_4$	ES+	8.42	301.0	30	168.0	10
9	Phenmedipham	$C_{16}H_{16}N_2O_4$	ES+	8.42	301.0	30	136.0	20
9	Propamocarb	$C_9H_{20}N_2O_2$	ES+	2.83	189.1	30	102.0	15
9	Propamocarb	$C_9H_{20}N_2O_2$	ES+	2.83	189.1	30	144.0	10
10	Carbendazim	$C_9H_9N_3O_2$	ES+	5.17	192.1	35	160.1	15
10	Carbendazim	$C_9H_9N_3O_2$	ES+	5.17	192.1	35	132.1	30

V. ORDERING INFORMATION

Product description	Part number
LC Multiresidue Pesticide Standards Kit	186007574
LCMS QC Reference Material	186006963
20 Pesticide Mix Standard	186006348
Quad LCMS QC Reference Material	186007362
LCMS Certified Amber Glass 12 x 32 mm Screw Neck Max Recovery Vial, with Cap and PTFE/silicone Septum, 2 mL Volume, 100/pkg	600000754CV

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